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Abstract: This paper deals with selecting control structures for a three-product Petlyuk (dividing-wall) column with an objective to achieve desired product purities with minimum use of energy (V). We consider four alternate control structures with and without the vapor split as a degree of freedom. This work also demonstrates the usefulness of the graphical Vmin diagram to visualize minimum boilup requirement and choose the appropriate control structure.

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The Editor,  
Chemical Engineering and Processing: Process Intensification

Dear Editor,

We are submitting herewith our **revised** manuscript entitled “Control structure selection for three-product Petlyuk (dividing-wall) column”, for your kind consideration.

We have responded to all the comments of the reviewers and made the corrections wherever necessary. We hope that the current version of the manuscript has been improved to the satisfaction of the reviewers. We will be happy to respond to any further comments/ queries.

We thank the reviewers for their feedback.

Thank you very much,

Sincerely yours,

Deeptanshu Dwivedi

# Control structure selection for three-product Petlyuk (dividing-wall) column

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## Abstract

This paper deals with selecting control structures for a three-product Petlyuk (dividing-wall) column with an objective to achieve desired product purities with minimum use of energy ( $V$ ). We consider four alternate control structures with and without the vapor split as a degree of freedom. This work also demonstrates the usefulness of the graphical  $V_{min}$  diagram to visualize minimum boilup requirement and choose the appropriate control structure.

*Keywords:* Energy Efficient Distillation, Thermally Coupled Distillation, Control Structure Design, Dividing-wall columns, Petlyuk Column

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## 1. Introduction

For three-product separations, the Petlyuk (see Figure 1 [23]) or divided-wall arrangements [14] offer significant savings in both energy and capital costs, as also shown by Cahn and DiMiceli [5], Stupin [28]. The German company, BASF has more than 100 dividing-wall columns [7]. However, operation and control is challenging and this paper proposes some new control schemes which are workable for varying feed composition disturbances.

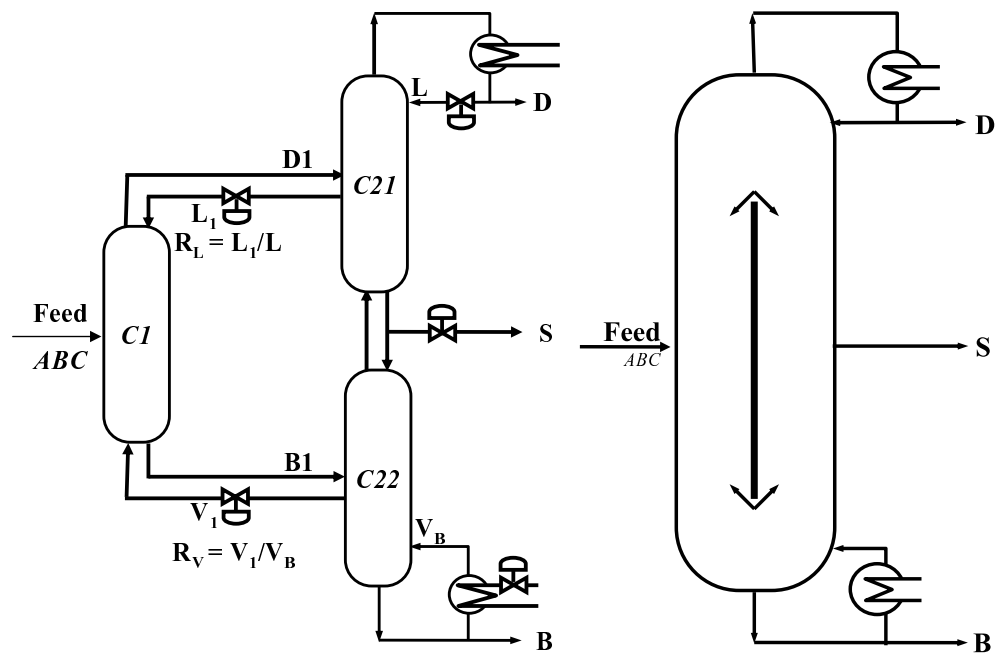
Halvorsen and Skogestad [11, 13] have developed a graphical tool, the “ $V_{min}$  diagrams”, to visualize the minimum energy requirement for sharp and non-sharp separations in conventional and thermally coupled columns. This tool can be used for designing such arrangements [7] and we will also demonstrate its use to give some insights into control and operation.

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(a) Implementation with three separate columns (b) Dividing-wall implementation with a side-product

Figure 1: Thermodynamically equivalent implementations of three-product Petlyuk column

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In terms of operation, several works have been published. Mutalib and Smith [20] reported simulation studies on the divided-wall columns. In their second work, Mutalib et al. [21] reported experimental studies conducted on a pilot plant and recommended a two point control of the system. Wolff and Skogestad [29] did a steady state study and operability analysis on a three-product Petlyuk column and conclude that the simultaneous specification of both impurities in the side-product is generally infeasible. Further, the liquid and vapor split ratios between pre-fractionator and the main column should be manipulated to get the optimal energy benefits. If the vapor split is not available as a degree of freedom, which is normally the case, one cannot control both ends of the prefractionator at the same time. Christiansen and Skogestad [6], Halvorsen and Skogestad [10] therefore proposed to use the liquid split to control the key impurity in the least pure end of the prefractionator. Ling and Luyben [18] explained that the liquid split valve ( $R_L$ ) must be manipulated and proposed a control structure with the use of four composition loops with the liquid split controlling the heavy key at the top stage of the prefractionator. In their second work, Ling and Luyben [19] studied the effectiveness of temperature control for BTX columns. Similar to Ling and Luyben [18], Kiss and Rewagad [15] and Rewagad and Kiss [24] suggested that control of the heavy key at the prefractionator top together with three composition loops in the main column may be sufficient to yield high-purity products and “implicitly” minimize the energy usage. Niggemann et al. [22] conducted simulation and experimental studies for separation of a mixture of fatty alcohols into three high-purity products. They reported that the heat transfer across the dividing wall can be a factor in design and operation. Lestak et al. [16] argued that in some cases the heat transfer across the dividing wall may decrease the overall energy consumptions. In non-beneficial regions however, the wall should be insulated. Some other works on the suitability of Model Predictive Control for dividing-wall columns have also been reported [24, 4, 1]. Ling et al. [17] suggested a control structure to avoid remixing of the intermediate component for optimal operation.

In this paper, we study the separation of a feed with components A (lightest), B and C (heaviest) in a Petlyuk column as shown in Figure 1. Note that the letter B is also used to denote the bottom product. To avoid confusion, we will use subscripts for components and superscripts for products. For example,  $x_A^D$  denotes the mole fraction of component A in product D.

With a given feed, the three-product Petlyuk column in Figure 1 has a total of five steady-state degrees of freedom, if we include an adjustable vapor

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9 split ( $R_V$ ). To obtain minimum energy operation, two of these degrees of  
10 freedom ( $R_L$  and  $R_V$ ) must be used to control the purity of the two “products”  
11 in the prefractionator (C1 in Figure 1), [10]. This leaves three degrees of  
12 freedom D, S and B in the main column (C21 and C22 in Figure 1), but we  
13 have four key impurities to control:  
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- 15 1. Heavy key or component B in product D ( $x_B^D$ )
- 16 2. Light key or component A in product S ( $x_A^S$ )
- 17 3. Heavy key or component C in product S ( $x_C^S$ )
- 18 4. Light key or component B in product B ( $x_B^B$ )

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22 In agreement with Wolff and Skogestad [29], we find that these four com-  
23 positions can not be specified independently, but we find that there is a possi-  
24 bility to over-purify one product, with the other products at their specifica-  
25 tions. The aim of this work is to find some simple single-loop (decentralized)  
26 PI control structures that are workable for large feed disturbances.  
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## 29 30 2. Case Study

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32 The data for the case study are given in Table 1. The process is modelled  
33 in Matlab using the simplifying assumptions of constant relative volatility  
34 and constant internal molar flows in column sections. This may seem unreal-  
35 istic but similar results are obtainable for real mixtures. The three hypothet-  
36 ical components A, B and C have relative volatilities similar to the mixture  
37 of ethanol, propanol and *n*-butanol. We assume constant pressure, negligible  
38 vapor holdup, a total condenser and equilibrium on all stages. We assume  
39 linearized liquid flow dynamics. Compared to the product purities given in  
40 Table 1, we have a large number of stages in each sub-column. This implies  
41 that the required energy is close to the minimum energy using an infinite  
42 number of stages. The nominal composition profiles are shown in Figure 2.  
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45 Figure 3 shows the  $V_{min}$  diagram for our A, B, C mixture with a liquid  
46 feed. The  $y$ -axis shows the normalized minimum boilup ( $V/F$ ) and the  $x$ -axis  
47 shows the net product withdrawal ( $D/F$ ) in a conventional two-product col-  
48 umn. The red-solid line is for the nominal equimolar feed and the blue-dashed  
49 line is for a feed composition disturbance where the ratio of components A  
50 and B is changed from 1:1 to about 4:1.  
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53 For Petlyuk arrangements, the minimum energy requirement to separate  
54 a multi-component feed is equal to the “most difficult binary separation”  
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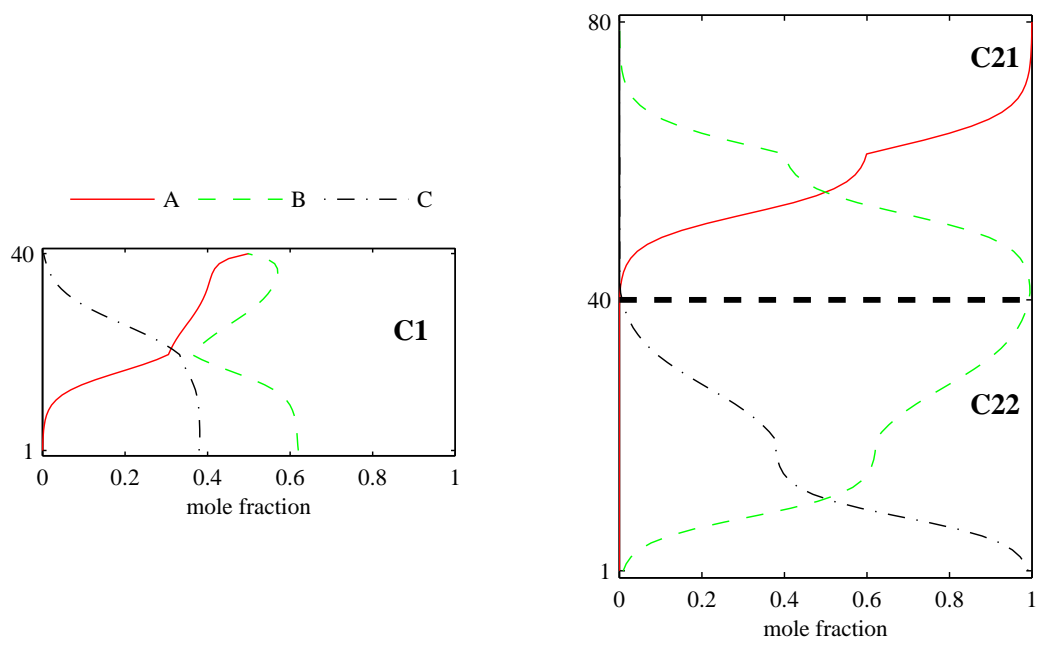


Figure 2: Nominal composition profiles of components: A (ethanol), B (propanol) and C (*n*-butanol) in sub-columns C1, C21 and C22

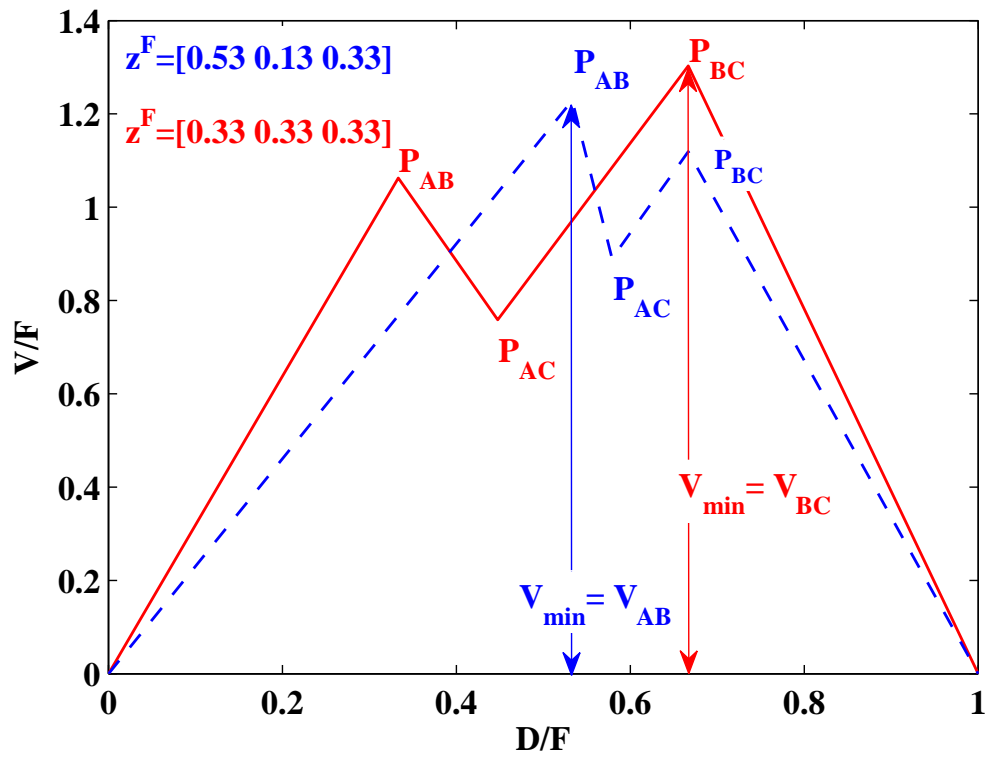


Figure 3:  $V_{min}$  diagrams for nominal equimolar feed (solid-red line) and for feed composition,  $z_5^F$  (mol%) = [53.33 13.33 33.33] (dashed-blue line). Relative volatilities,  $\alpha = [4.2 \ 2.1 \ 1]$  and feed liquid fraction,  $q_F = 1$ .



Table 1: Input data and nominal conditions for the three-product Petlyuk column model

Relative volatilities [A, B, C]	[4.2 2.1 1]
Number of stages in C1	20+20
Number of stages in C21	20+20
Number of stages in C22	20+20
Nominal feed flow rate (F)	1 kmol/min
Nominal feed composition [A, B, C]	[33.3 33.3 33.3] (mol %)
Nominal liquid reflux (L)	1.0033 kmol/min
Nominal boilup (V)	1.3381 kmol/min
Nominal distillate flow rate (D)	0.3348 kmol/min
Nominal bottom flow rate (B)	0.3333 kmol/min
Nominal side-product (S)	0.3318 kmol/min
Nominal liquid split ( $R_L$ )	0.3465
Nominal vapor split ( $R_V$ )	0.5982
Nominal purity of distillate ( $x_A^D$ )	99.5 (mol %)
Nominal purity of side-product ( $x_B^S$ )	99.45 (mol %)
Nominal light impurity of side-product ( $x_A^S$ )	0.05 (mol %)
Nominal heavy impurity of side-product ( $x_C^S$ )	0.5 (mol %)
Nominal purity of bottom product ( $x_C^B$ )	99.5 (mol %)
Nominal heavy impurity of prefractionator top ( $x_C^{D1}$ )	0.29 (mol %)
Nominal light impurity of prefractionator bottoms ( $x_A^{B1}$ )	0.08 (mol %)

[8, 12].

$$V_{min, Petlyuk} = \max(V_{AB}, V_{BC}) \quad (1)$$

Here,  $V_{AB}$  and  $V_{BC}$  are the vapor flows corresponding to the peaks  $P_{AB}$  and  $P_{BC}$ , respectively, in Figure 3. For the nominal case with an equimolar feed, the  $P_{BC}$  peak is the highest. This implies that nominally, B/C is the most difficult binary split in terms of energy usage. However, for the feed composition disturbances, the A/B split becomes the most difficult split. Depending on whether A/B or B/C is the more difficult split, we will have excess energy in one of the sections (C21 or C22, respectively) of the main column. Therefore, there is a possibility to over-purify in one of these two sections with only minor penalty in terms of energy usage. When A/B is the more difficult split, we may choose to over-purify the bottom product or the

heavy component (C) in the side-product, and when B/C is the more difficult split, we may choose to over-purify the top product or the light component (A) in the side-product.

### 3. Control Structures for three-product Petlyuk column

#### 3.1. Control Objectives

We assume that the operational objective for a given feed is to minimize the energy consumption subject to satisfying purity constraints on the three products. That is, the cost function to be minimized is:

$$J = \text{energy} (V) \tag{2}$$

A more general cost function would be to take into account also the prices and amounts of products and of heat input and cooling, but this is not considered here. The purity constraints are assumed to be given in terms of the amount of key impurity in each product:

$$\begin{array}{ll}
 \text{Impurity in top product} & (D) : x_B^D \leq x_{B,s}^D \quad (= 0.5\%) \\
 \text{Light Impurity in side product} & (S) : x_A^S \leq x_{A,s}^S \quad (= 0.5\%) \\
 \text{Heavy Impurity in side product} & (S) : x_C^S \leq x_{C,s}^S \quad (= 0.5\%) \\
 \text{Impurity in bottom product} & (B) : x_B^B \leq x_{B,s}^B \quad (= 0.5\%)
 \end{array} \tag{3}$$

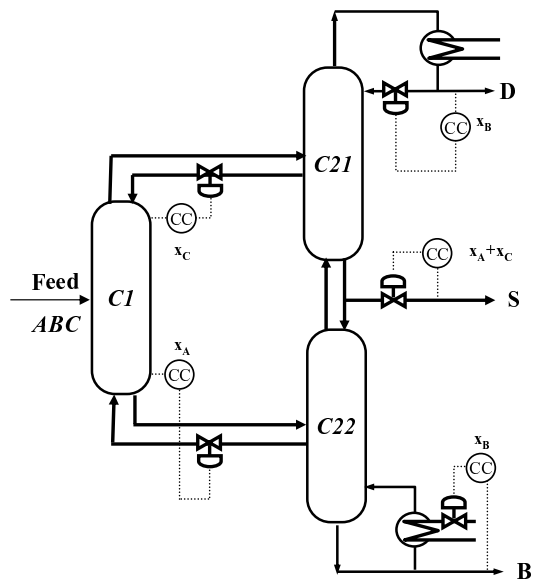
Note that the side-product contains the two impurities (A and C). The resulting minimum purity of the main component in each product is 99.5% for the distillate, 99.0% for the side-product and 99.5% for the bottom product.

We assume that these four constraints are always optimally active, meaning that the energy consumption (J=V) is minimized by having equality for the four specifications in (3).<sup>1</sup> However, as discussed by Wolff and Skogestad [29], their may be “holes” in the operating range making it difficult or

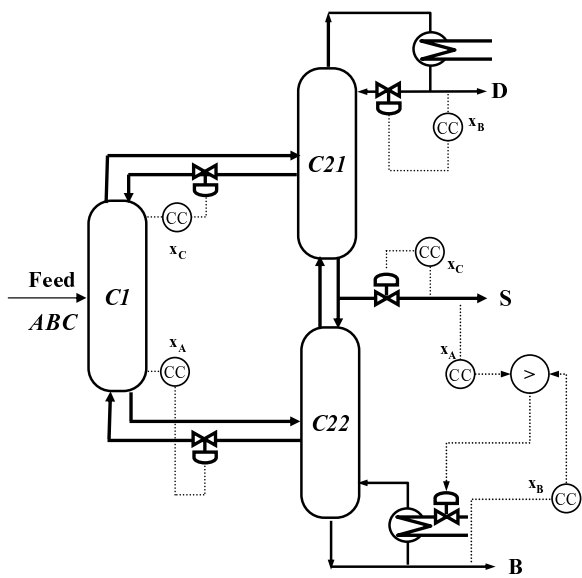
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<sup>1</sup>Alstad et al. [3] have shown that in some cases it may be possible to obtain some minor energy savings by over-purifying the top product (for the case when B/C is the difficult split) or the bottom product (for the case when A/B is the difficult split), because this simplifies the separation in the side-product by increasing the amount of component B in the side-product. However, the effect is small, and we here assume that all product purity specifications are optimally active.

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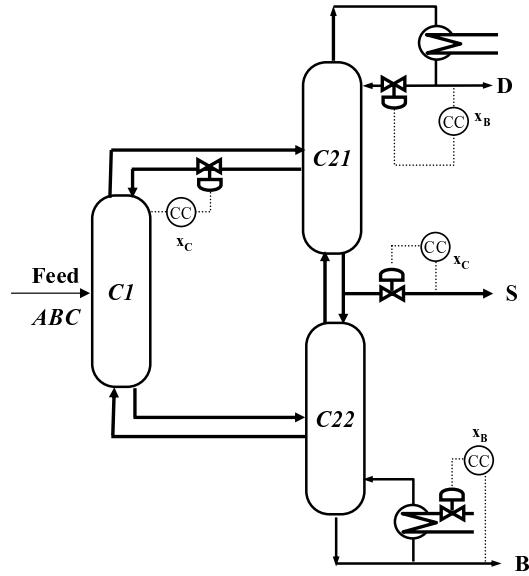
(a) CS1: control of  $x_A+x_C$  in sidestream (*Not recommended for dynamic reasons*).



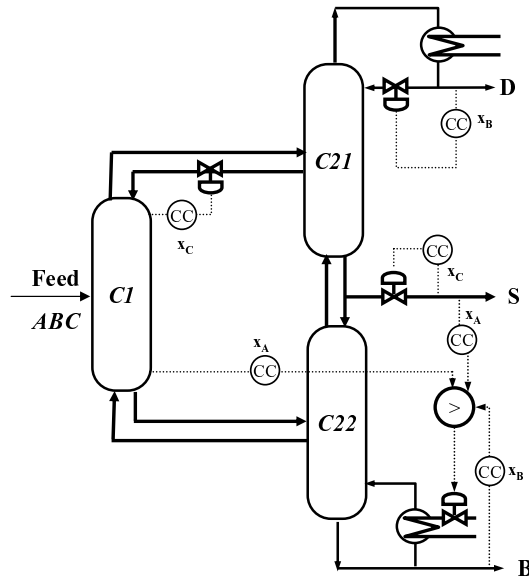
(b) CS2: control of  $x_C$  in sidestream and max-selector to avoid  $x_A$  in side stream (*Recommended for all feed compositions*).

Figure 4: Control Structures *with* active use of vapor split ( $R_V$ ).

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(a) CS3: No control of  $x_A$  in sidestream and in bottom of prefractionator [18] (*Recommended A/B is the easy split*).



(b) CS4: Max-selector to avoid large  $x_A$  in sidestream and in bottom of prefractionator (*Recommended for all feed compositions*).

Figure 5: Control Structures *without* use of vapor split ( $R_V$ ).

impossible in practice to control all four compositions simultaneously. Instead of controlling four compositions, we therefore, consider two options for controlling three compositions:

1. *Option I*: Control the total impurity in the side stream  $x_A^S + x_C^S$  (as done in structure CS1, see Figure 4(a)).
2. *Option II*: Over-purify one of the products (as done in structure CS2, see Figure 4(b)). This will come at some loss in terms of energy (V) but as discussed in the previous section, the loss may be very small.

To satisfy three of the specifications in (3) using “*Option I*” or “*Option II*”, we need three degrees of freedom (e.g., L, S and V).<sup>2</sup> There are then two unconstrained degrees of freedom (e.g.,  $R_L$  and  $R_V$ ) left for minimizing the energy ( $J=V$ ) and these need to be translated to control objectives.

One may think that a good approach would be to set the energy input (boilup) V directly and try to minimize it, but this is not a workable solution as it may lead to infeasibility because the product specifications can not be met if V is set lower than its optimal (minimum) value. The concept of “self-optimizing control” [25] provides a general theory for obtaining good control objectives. In this paper, we assume that good self-optimizing variables are the two “product” compositions in the prefractionator (C1) [10]. This is reasonable because the prefractionator will then operate very close to its “preferred” split. Thus, we use the following controlled variables (specifications):

$$\begin{aligned}
 \text{Heavy key (C) in top “product” of prefractionator (D1)} & : x_C^{D1} = x_{C,s}^{D1} \\
 \text{Light key (A) in bottom “product” of prefractionator (B1)} & : x_A^{B1} = x_{A,s}^{B1}
 \end{aligned}
 \tag{4a}$$

### 3.2. Setpoints for the controlled variables

The setpoints for the compositions in the main column are determined by the product specification as given in (4a). For the prefractionator, the setpoint values in (4a) should ideally be the optimal values that minimize the energy consumption (V). The optimal value may vary depending on the feed

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<sup>2</sup>It may seem strange that the cost variable  $J=V$  is also a degree of freedom, but this is correct.

composition and product purity specifications (for D, S and B), but since the prefractionator performs the “easy” A/C-split, we usually have enough stages to “over-purify” in the prefractionator, with only a slight penalty in terms of increased energy (V). Some over-purification in prefractionator is also good from operational perspective, as we can then avoid the problem of infeasibility of purity specifications in the main column, in the event of disturbances. This is equivalent to the introducing a “back-off” from the self-optimizing variable as also described by Govatsmark and Skogestad [9].

In our case study, we use for in all simulations and control studies (and for the nominal point) the following specifications for the prefractionator:

$$\begin{aligned} x_{C,s}^{D1} &= 0.29\% \\ x_{A,s}^{B1} &= 0.08\% \end{aligned} \tag{4b}$$

How did we arrive at these values? This is quite a long story, but let us first repeat that the exact values are not critical because the A/C split performed in the prefractionator is relatively easy. We started by obtaining the optimal solution for the nominal feed composition: For the constraints in (3) and the objective (2) we found a minimum boilup (V) of 1.3322 kmol/min with all the four impurity constraints in (3) optimally active. However, this “optimal” solution has some undesirable features. First, we find that the amount of component C over the top in the prefractionator is high (0.83%) given that we want less than 0.5% C in the side-product. Second, this “optimal” solution does not over-purify any of the products, in spite of the fact that we know from the  $V_{min}$  diagram in Figure 3 (where we see that A/B is the easier split at nominal feed conditions) that we can over-purify either the top product or the side product with almost no extra energy (V). In some sense we can say that the “optimal” solution is going against the “natural” product distribution, which is to over-purify one of the products. Which product should we over-purify? This is mainly an operational issue, and we choose to over-purify A in the side stream. This makes control of the side stream easier, since we at least nominally need not consider the amount of A in the side-product. So we reduced the impurity of A in the side stream from its specification of 0.5% to 0.1%, and re-optimized the operation. The resulting boilup (V) increased only marginally from 1.3322 kmol/min to 1.3325 kmol/min, so we can indeed over-purify for free. The resulting optimal values for the “product” compositions in the prefractionator were:  $x_{C,opt}^{D1}=0.58\%$  and  $x_{A,opt}^{B1}=0.16\%$ . However, this is for the nominal feed composition, and to handle feed compositions changes, we choose divide these values by a factor 2

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9 and ended up with the final specifications in (4b). Using the specifications in  
10 (4b), resulted in a slight further increase in boilup (V) from 1.3325 kmol/min  
11 to 1.3381 kmol/min, and it gave a further reduction of A-impurity in the side  
12 stream from 0.10% to 0.05%. The final nominal flows and purities are given  
13 in Table 1.  
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15 So far, we have assumed that the vapor split ( $R_V$ ) is a degree of freedom.  
16 Unfortunately, this is not the case with most (if not all) Petlyuk columns in  
17 operation. Thus, for practical columns, where  $R_V$  is not a degree of freedom,  
18 we generally need to use extra energy, and the result is that we will get  
19 over-purification (inequality) for yet one more of the purities in (3) and (4).  
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### 22 3.3. Control Structures

23 With this introduction to the control objectives and setpoints, we now  
24 consider four alternative control structures; CS1 and CS2 (Figure 4) are  
25 for the next-generation dividing-wall columns where the vapor split ( $R_V$ ) is  
26 available as a degree of freedom, whereas CS3 and CS4 (Figure 5) are for the  
27 more realistic case today where  $R_V$  is not a degree of freedom.  
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30 Note that in all cases, we use the standard “LV-configuration” where the  
31 distillate flow (D) is used for level control of the condenser and the bottoms  
32 flow (B) is used for level control of the reboiler, so that reflux (L) and boilup  
33 (V) remain as degree of freedom for composition control.  
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#### 36 3.3.1. Control Structure 1 (CS1)

37 In this structure, we use “Option I” and control the sum of the impurities  
38 ( $x_A^S + x_C^S$ ) with the side-product (S). Since the vapor split ( $R_V$ ) is available for  
39 manipulation, we then have two degrees of freedom left and can control both  
40 “products” in the prefractionator (see 4(a)). This will guarantee operating  
41 the prefractionator at its preferred split [12]. For control loop pairings, we  
42 use the most obvious “close-by” manipulated variables as shown in 4(a).  
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45 This scheme is workable at steady state but performs poorly for some  
46 feed disturbances. The reason is that the sign of the initial gain of the molar  
47 flow rate of side-product on the two key impurities is opposite. Depending  
48 upon the dominant impurity in the side-product, the input (S)-output ( $x_A^S +$   
49  $x_C^S$ ) relationship will change, making it very difficult to work under transient  
50 conditions. We will demonstrate using closed-loop simulations that structure  
51 CS1 has poor dynamic response properties to feed composition disturbances  
52 and CS1 is therefore *not* recommended.  
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### 3.3.2. Control Structure 2 (CS2)

In structure CS2, we use “*Option II*” where we overpurify one of the products. We use the side-product (S) to control the heavy key impurity ( $x_C^S$ ). This means that the amount of light component, A ( $x_A^S$ ) is left uncontrolled which is acceptable as long as it is over-purified. However, if  $x_A^S$  becomes large then we need to increase the vapor flow in section C21 and instead overpurify the bottom product. To achieve this we pair the boilup (V) with two composition controllers (both  $x_B^D$  and  $x_A^S$ ) and use a max-selector. This means that one of the two products (bottoms or side-product) will be over-purified for any disturbance. However, as explained earlier this will only slightly increase the energy usage (V).

### 3.3.3. Control Structure 3 (CS3)

We also study two structures for the case when the vapor split is not available as a degree of freedom. Control structure CS3 in Figure 5(a), has been suggested by Ling and Luyben [18] and a similar control structure was reported by Alstad [2, Chapter 9] and Kiss and Rewagad [15]. Since the vapor split is not available for control, the prefractionator column C1 can have only one-point control and the light component (A) at C1 bottoms is left uncontrolled. In the main column, the side-product is paired with the heavy key (C) while the light key (A) in side-product remains uncontrolled. This is acceptable as long as there is little light component A in the side-product (over-purified). As confirmed in the simulations, this structure fails if the feed composition is such that A/B split is the most difficult one.

### 3.3.4. Control Structure 4 (CS4)

This is an improvement of CS3, which is workable also when A/B is the more difficult split. It is based on the same idea as structure CS2, but the boilup now also looks after the amount of A in the prefractionator C1 bottoms. To ensure sufficient vapor flow, we use a maximum-select controller and pair the boilup with the largest boilup resulting from controlling the following three impurities:

1. Component A in bottom of prefractionator ( $x_A^{B1}$ )
2. Component A in side-product ( $x_A^S$ )
3. Component B in bottom-product ( $x_B^B$ )

This implies that two of these compositions will be overpurified at any given time, and it is expected that the energy usage (V) may be large for some disturbances.



#### 4. Closed loop simulation results

Table 2: Summary of closed-loop composition responses using different control structures (superscript numbers refer to corresponding Figure numbers)

Disturbance	CS1	CS2	CS3	CS4
Feed, +20 %	OK <sup>6(a)</sup>	OK <sup>7(a)</sup>	OK <sup>8(a)</sup>	OK <sup>9(a)</sup>
Feed, -20 %	OK <sup>6(b)</sup>	OK <sup>7(b)</sup>	OK <sup>8(b)</sup>	OK <sup>9(b)</sup>
$z_1^F$ (mol%) = [ <b>13.3 53.3</b> 33.3]	Poor <sup>6(c)</sup>	OK <sup>7(c)</sup>	OK <sup>8(c)</sup>	OK <sup>9(c)</sup>
$z_2^F$ (mol%) = [ <b>13.3</b> 33.3 <b>53.3</b> ]	OK	OK	OK	OK
$z_3^F$ (mol%) = [33.3 <b>53.3</b> <b>13.3</b> ]	Poor <sup>6(d)</sup>	OK <sup>7(d)</sup>	OK <sup>8(d)</sup>	OK <sup>9(d)</sup>
$z_4^F$ (mol%) = [33.3 <b>13.3</b> <b>53.3</b> ]	Poor <sup>6(e)</sup>	OK <sup>7(e)</sup>	Fail <sup>8(e)</sup>	OK <sup>9(e)</sup>
$z_5^F$ (mol%) = [ <b>53.3</b> <b>13.3</b> 33.3]	OK <sup>6(f)</sup>	OK <sup>7(f)</sup>	Fail <sup>8(f)</sup>	OK <sup>9(f)</sup>
$z_6^F$ (mol%) = [ <b>53.3</b> 33.3 <b>13.3</b> ]	OK	OK	Fail	OK

<sup>a</sup> OK: Closed-loop stable and purities all products are either restored/over-purified and the transient responses are not very severe

<sup>b</sup> Fail: Closed-loop stable but purity of side-product is not maintained ( $x_B^S$  dropped considerably)

<sup>c</sup> Poor: Although steady state purities may be restored, the transient response is poor and shows valve saturation

<sup>d</sup> Nominal feed rate:  $F=1$  kmol/min

Nominal feed composition,  $z_F$  (mol%) = [33.3 33.3 33.3]

The four control structures were simulated for the nominal case, for a  $\pm 20$  % feed rate change and for six feed composition disturbances of which four cases are shown in Figures 6 to 9. All the control structures could handle the feed rate disturbance of  $\pm 20$  % but for the feed composition disturbances, some responses using structures CS1 and CS3 were poor.

Nominally, the column is operated at a point where both splits A/B and B/C are “difficult” and none of the products are over-purified. However, for feed composition disturbances,  $z_1^F$ ,  $z_2^F$  and  $z_3^F$ , the B/C split is the most difficult one and for feed composition disturbances  $z_4^F$ ,  $z_5^F$  and  $z_6^F$ , the A/B split is more difficult. The results of the closed-loop simulations feed rate and all six compositions are summarized in Table 2 and we see that structure CS3 fails when the A/B split is more difficult.

Simple decentralized proportional-integral (PI) controllers with SIMC tuning [25] were used. Step changes in the manipulated variables were made

Table 3: SIMC tuning parameter ( $\tau_C$ ) used in the four control structures <sup>a,b</sup>

Loop	CS1	CS2	CS3	CS4
R <sub>L</sub>	10 min	10 min	10 min	40 min
R <sub>V</sub>	40 min	40 min	–	–
L	20 min	10 min	10 min	40 min
S	80 min	40 min	40 min	10 min
V <sub>B</sub>	10 min	40 & 40 min <sup>a</sup>	40 min	40, 40 & 10 min <sup>b</sup>

<sup>a</sup>  $\tau_C$  for V<sub>B</sub> paired with B in reboiler &  $\tau_C$  for V<sub>B</sub> paired with A in side-product respectively

<sup>b</sup>  $\tau_C$  for V<sub>B</sub> paired with B in reboiler,  $\tau_C$  for V<sub>B</sub> paired with A in side-product &  $\tau_C$  for V<sub>B</sub> paired with A in sub-column C1 bottoms respectively

to identify the input-output steady state gain and effective time delay. The SIMC tuning parameter,  $\tau_C$  was selected to get a smooth response (see Table 3). Note that the tuning was straight forward. The energy loop involving the maximum-select controllers were detuned for a smooth response.

In addition, logarithmic transformations of compositions were used to reduce the effect of non-linearity [26, 27]. Therefore, the controlled composition variables are actually  $\ln x_i$ , where  $x_i$  is the key impurity being controlled.

#### 4.1. Simulation of structure CS1

Figure 6 shows closed-loop responses using CS1 for a  $\pm 20\%$  feed rate changes and feed composition disturbances. We use a semi-log scale to plot the compositions of the key impurities in the main products D, S and B. The side-product has two key impurities, A and C. We observe that the closed-loop responses for feed disturbances,  $z_1^F$  and  $z_3^F$  (Figures 6(c) and 6(d)) show poor transient responses. After a long time (not shown in simulations), the impurities are restored to their steady-state values. However, this structure is not recommended, as during the transient conditions, the inputs saturate and there are very large changes in the product compositions.

#### 4.2. Simulation of structure CS2

Control structure CS2 shows good dynamic responses for the  $\pm 20\%$  feed rate changes and the feed composition disturbances as shown in Figure 7. The steady state impurities of the products are better than the specifications

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9 (3). For feed compositions when the B/C split is more difficult (Figures 7(c)  
10 and 7(d)), the light impurity (A) in side-product is not controlled and is  
11 over-purified. For feed compositions when A/B is the more difficult split,  
12 the maximum-select controller pairs the boilup with the light key in side-  
13 product and the bottom product is over-purified (Figures 7(e) and 7(f)). Note  
14 that for these cases, both key impurities in the side-product are controlled  
15 simultaneously.  
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#### 18 19 4.3. Simulation of structure CS3

20 We next consider the case when the vapor split ( $R_V$ ) is not a degree of  
21 freedom. Control structure CS3 does not attempt to control A in the side  
22 product and is workable for cases where B/C is the most difficult split (dis-  
23 turbances  $z_F^4$  and  $z_F^5$ , see Figures 8(c) and 8(d)). However, for disturbances  
24 when A/B is the more difficult split (Figures 8(e) and 8(f)). We have “break-  
25 through” of A in the bottom of the prefractionator (see, for example, Figure  
26 10) and the impurity constraint ( $x_A^S, x_C^S < 0.5\%$ ) is violated both dynamically  
27 and at steady-state.  
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#### 30 31 4.4. Simulation of structure CS4

32 Figure 9 shows closed-loop responses using control structure CS4. The  
33 product purities of all products can be controlled within the constraints (3)  
34 at steady state in all cases. When A/B is the more difficult split, the boilup  
35 is not paired with the bottom light key and therefore the bottom product is  
36 over-purified (Figures 9(e) and 9(f)).  
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### 40 41 5. Analysis of energy usage

42 We have found in the simulations that control structures CS2 and CS4  
43 give good composition control in all cases, but in addition we want the struc-  
44 tures to achieve minimum energy usage, or at least close to minimum energy  
45 usage. We have plotted the energy usage (V) in all simulations, but to say  
46 how good it is we need to compare with the minimum energy usage for the  
47 various feed compositions. This is shown in Table 4 where we compare the  
48 steady-state energy usage for control structures CS2 and CS4 with the opti-  
49 mal for each case, that is, with and without the vapor split ( $R_V$ ) as a degree  
50 of freedom, respectively. The results show that control structure CS2 is close  
51 to the optimal for all feed compositions, with a maximum energy loss of  
52 1.01 % for feed composition  $z_6^F$ . Control structure CS4 is also close to the  
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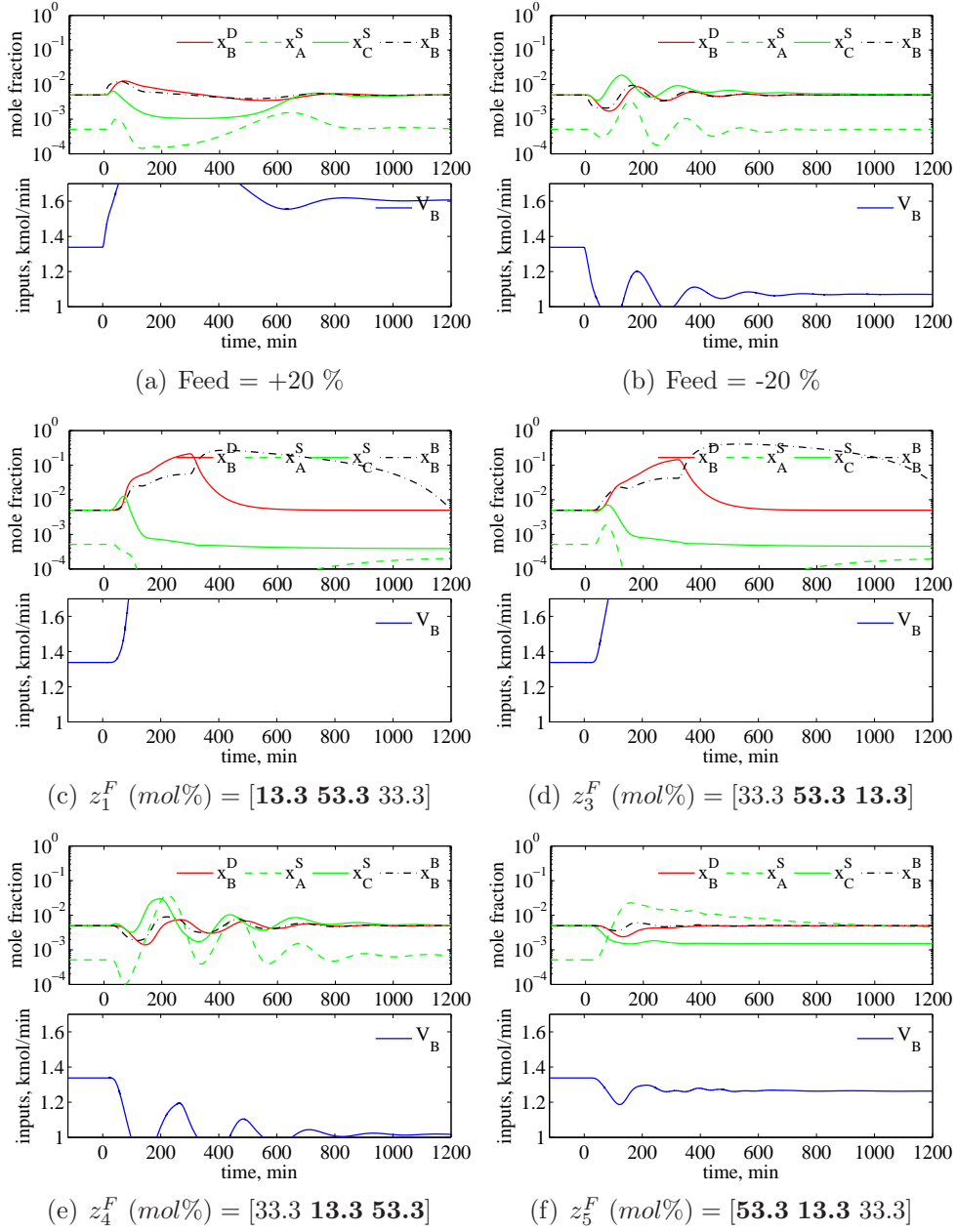


Figure 6: CS1: Closed-loop results for feed rate and composition disturbances (Not acceptable for feed composition disturbance  $z_1^F$ ,  $z_3^F$  and  $z_4^F$  as the transient response is poor).

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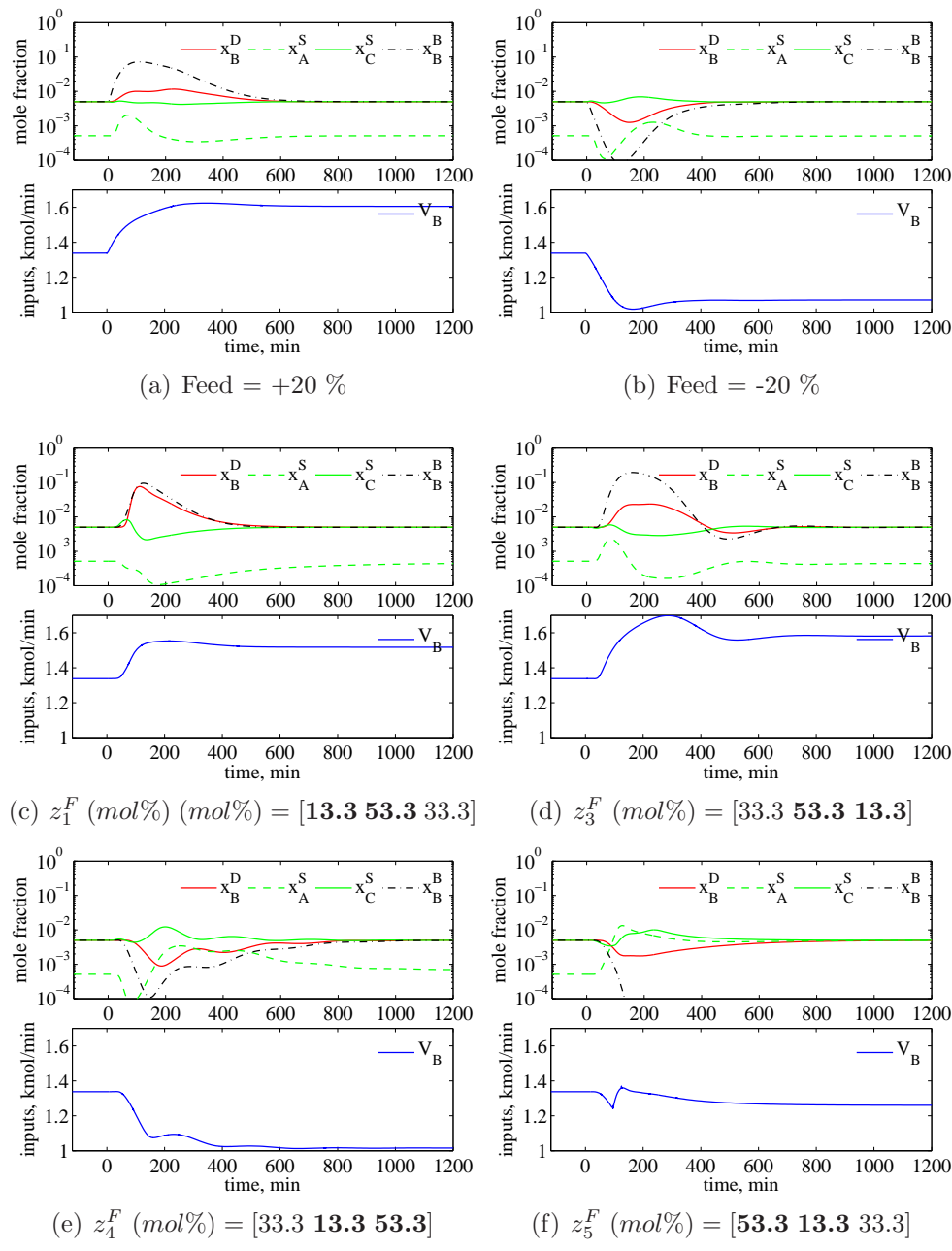


Figure 7: CS2: Closed-loop results for feed rate and composition disturbances (Acceptable for all disturbances).

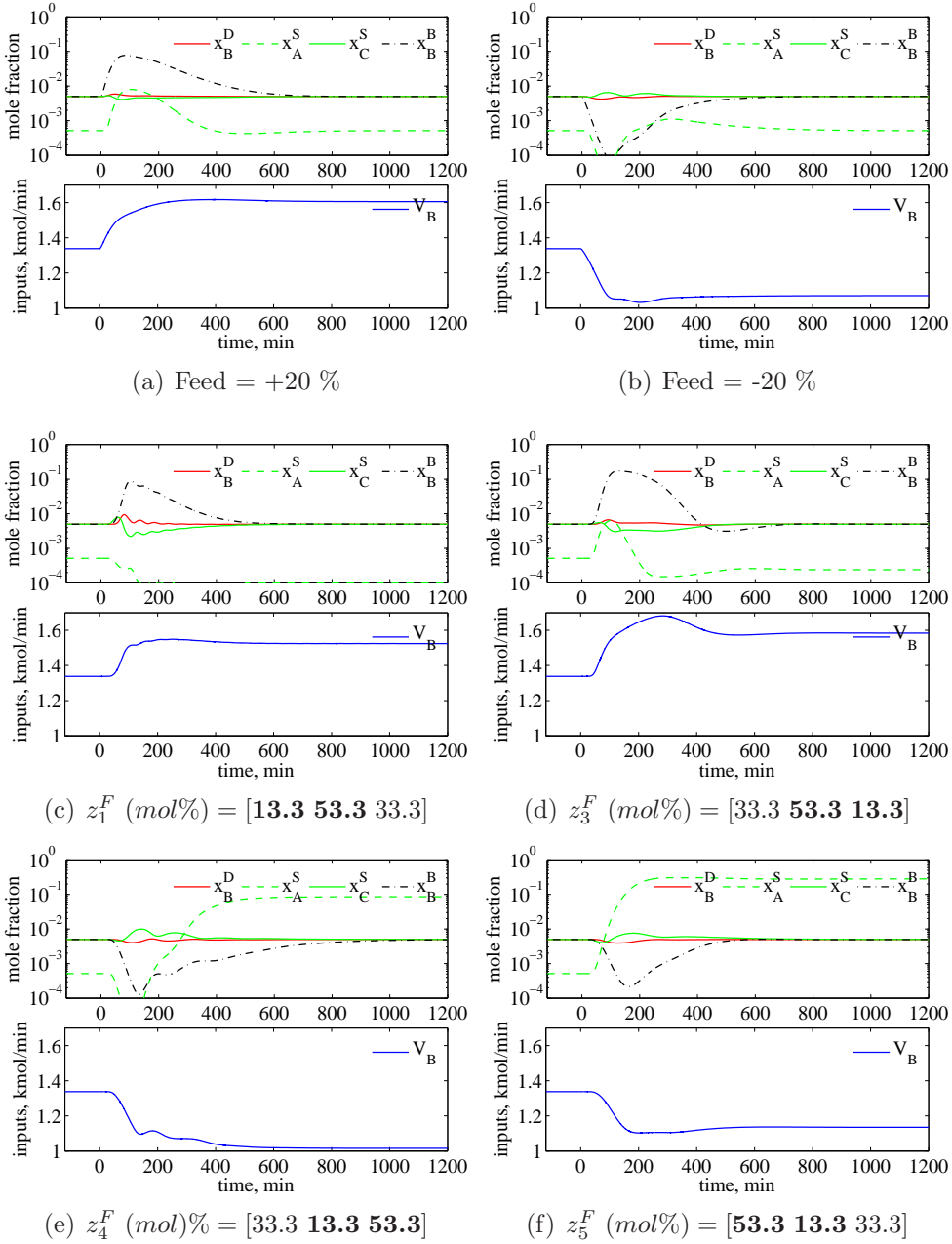


Figure 8: CS3: Closed-loop results for feed rate and composition disturbances (Not Acceptable for disturbances  $z_4^F$  and  $z_5^F$  as  $x_A^S$  goes out of bounds).

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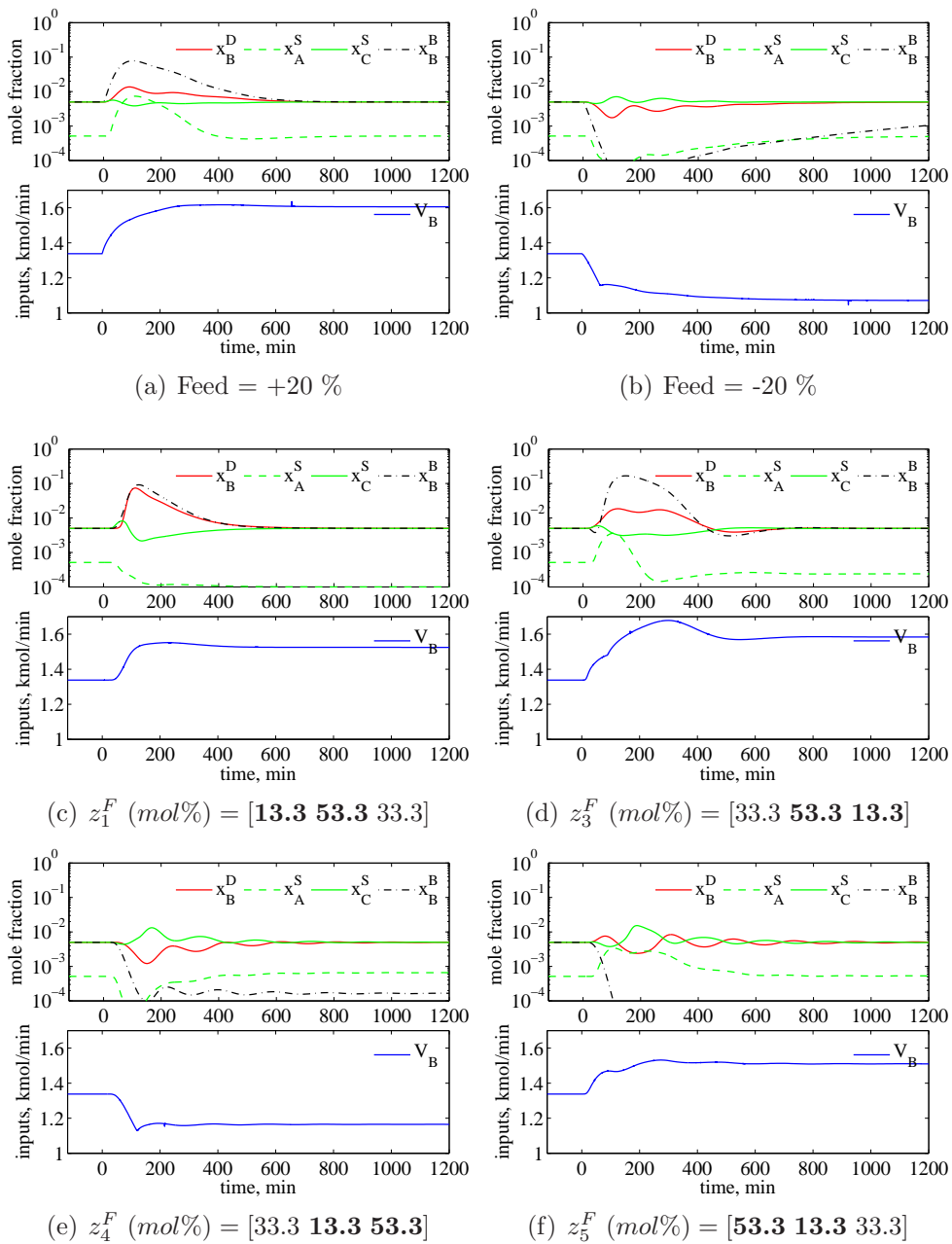


Figure 9: CS4: Closed-loop results for feed rate and composition disturbances (Acceptable for all disturbances).

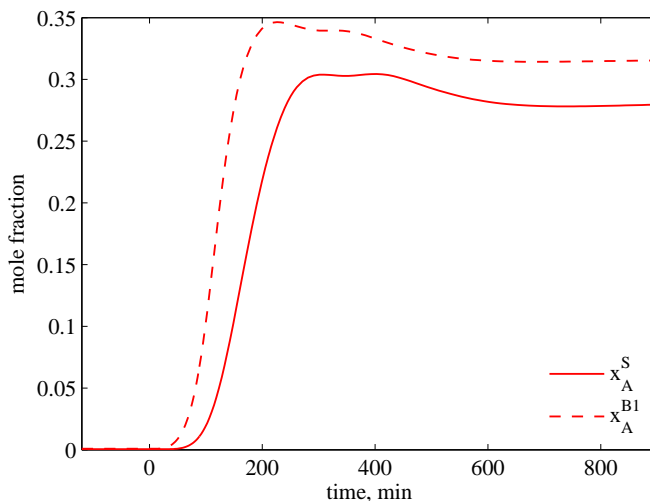


Figure 10: Failure of control structure CS3 for feed composition disturbance  $z_5^F$  (mol%) = [53.3 13.3 33.3] caused by breakthrough of component in bottoms of prefractionator ( $x_A^{B1}$ ) resulting in contaminated side product ( $x_A^S$ ).

optimal for all feed compositions, with a maximum energy loss of 2.27% for feed composition  $z_5^F$ . Note that the optimal energy usage is generally higher for structure CS4 than for CS2 (up to about 19.88% for  $z_5^F$ ), but this is an inevitable loss caused by operating with a fixed vapor split ( $R_V$ ). The reason for the (albeit small) energy losses for control structures CS2 and CS4 is mainly because the prefractionator is not operating quite optimally, that is, the prefractionator setpoints in (4b) are not the optimal ones as explained earlier in Section 3.2. This is also why the energy usage is 0.42 % above the minimum even for the nominal feed composition.

## 6. Discussion

### 6.1. Change in difficult split

Figure 3 shows how the  $V_{min}$  diagram depends on the feed composition. As explained earlier, the minimum boilup for sharp separation is set by the “most difficult binary split”, which are given in Figure 3 by the peaks  $P_{AB}$  and  $P_{BC}$ . For the nominal feed (red solid line), the peak  $P_{BC}$  is highest. This implies that the B/C split is more difficult. It is then acceptable to leave A uncontrolled in the side stream as in structure CS3. However, for a feed



Table 4: Energy usage at steady state for control structures CS2 and CS4 as compared against optimum energy usage with and without the vapor split ( $R_V$ ) for different feed composition disturbances.

Disturbance	Boilup (V), kmol/min			
	<i>with</i> $R_V$		<i>without</i> $R_V$	
	optimal	CS2	optimal	CS4
$z_1^F$ (mol%) = [ <b>13.3</b> <b>53.3</b> 33.3]	1.5070	+0.7 %	1.5072	+1.2 %
$z_2^F$ (mol%) = [ <b>13.3</b> 33.3 <b>53.3</b> ]	1.2528	+0.33 %	1.2551	+0.37 %
$z_3^F$ (mol%) = [33.3 <b>53.3</b> <b>13.3</b> ]	1.5713	+0.68 %	1.5722	+0.76 %
$z_4^F$ (mol%) = [33.3 <b>13.3</b> <b>53.3</b> ]	1.0151	+0.06 %	1.1434	+1.88 %
$z_5^F$ (mol%) = [ <b>53.3</b> <b>13.3</b> 33.3]	1.2571	+0.23 %	1.4769	+2.27 %
$z_6^F$ (mol%) = [ <b>53.3</b> 33.3 <b>13.3</b> ]	1.4533	+1.01 %	1.6406	0.87 %
$z^F$ (mol%) = [33.3 33.3 33.3]	1.3325	+0.42 %	1.3325	+0.42 %

composition making A/B the more difficult split (blue dashed line in Figure 3), the boilup should be increased, for example, using a selector to avoid A in the bottoms of the main column section C21 (A/B split) and as well as bottom of the prefractionator (A/C split, see Figure 10).

The magnitude of feed composition disturbance in this study is large. However, simulations show that structure CS3 fails and there is a breakthrough of light impurity (A) in the side product also for smaller feed disturbances. The reason is that the nominal operating point is quite close to a region where A/B may become the more difficult split.

### 6.2. Multivariable Control (MPC)

In this work, we have studied performance of decentralized control schemes based on PI-controllers and max-selectors as this is the preferred solution in industry, whenever it is found to be workable. We found that its performance is acceptable, but tuning the controllers was difficult in some cases. Thus, this may be a case where multivariable control (e.g. MPC) should be considered to reduce interactions and improve performance.

One may think that the max-select controllers can easily be replaced by a constrained multivariable controllers, like MPC. However, a more careful evaluation reveals that this is not so clear, because when we switch using the PI-controllers, we use controllers tuned in different operating regions, for

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9 example, with and without A in the side product. Thus, to get acceptable  
10 control with MPC, one probably would need to include model information  
11 from different operating regions, which may difficult to handle in a conven-  
12 tional linear MPC framework. Possibly, this could be a case where non-linear  
13 MPC based on physical models may be the preferred solution.  
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### 16 6.3. Other control structures

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18 In principle, there are many other possible control structures with selec-  
19 tors, in addition to CS2 and CS4, but these have not been studied. To see  
20 this, note that we are attempting to control *six* compositions, which include  
21 *two* for the two “products” in the prefractionator and *four* for the three prod-  
22 ucts in the main column, see (3) and (4). However, we only have *five* degrees  
23 of freedom for the case when  $R_V$  is a manipulated variable, and *four* degrees  
24 of freedom for the case when  $R_V$  is fixed during operation, respectively. Thus,  
25 we have too few degrees of freedom to control all *six* compositions and to  
26 satisfy the *six* specifications we need to overpurify some products. For the  
27 case when  $R_V$  is fixed, we are lacking two degrees of freedom and we propose  
28 in control structure CS4 to always control *three* of the compositions, and to  
29 overpurify *two* of the remaining *three* compositions using a selector. How-  
30 ever, it is not given which *three* compositions to include in the selector, and  
31 it is not given that boilup should be used in the selector. Specifically, for the  
32 split A/B we may choose to overpurify  $x_B^D$  (B in distillate) rather than  $x_A^S$  (A  
33 in sidestream), and for the split B/C we may choose to overpurify  $x_C^S$  (C in  
34 side stream) rather than  $x_B^B$  (B in bottom). Similarly, for the prefractionator,  
35 we may for the split A/C choose to overpurify  $x_C$  in the top rather than  $x_A$   
36 in the bottom. Some of these alternatives may be worthwhile considering,  
37 in particular, if overpurification of some product is desirable, whenever possi-  
38 ble. Nevertheless, of all these possible alternative structures, it seems that  
39 structure CS4 is a good choice, mainly because the boilup (V) has a direct  
40 effect on the three compositions used by the selector, and because the three  
41 remaining manipulated variables have a direct effect on the three remaining  
42 compositions. Indeed, it was found to give good composition control with  
43 close to minimum energy usage for a wide range of feed composition changes.  
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## 53 7. Conclusions

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55 In this work, we study decentralized control structures when the objective  
56 is to achieve desired purities for the three products with minimum use of  
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9 energy ( $V$ ). For the case where the vapor split ( $R_V$ ) is a degree of freedom,  
10 we propose to use structure CS2 as shown in Figure 4(a). It will generally  
11 lead to overpurification of either the side stream or bottom product, but this  
12 will cost very little in terms of extra energy usage. For the more realistic  
13 case where the vapor split is not a degree of freedom, the energy usage  
14 will be higher for some disturbances. This is inevitable, but otherwise the  
15 proposed structure CS4 (see Figure 5(b)) achieves the desired purities with  
16 use of minimum energy. The simpler structure CS3 may be used instead of  
17 CS4 for cases where the A/B split is relatively simple so that we always have  
18 low concentration of A (“overpurification”) in the side stream.  
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## Response to reviewers' comments

### *Reviewer # 1:*

In spite of some remarks, the article is well written and provides a continuation to a series of papers of the same research team on these particular distillation columns. It can be published after some correction. The reviewer simply regrets that, probably because of industrial habits, simple PIs controllers are still preferred when MPC would provide very easily efficient solutions in a multivariable framework with natural handling of constraints and with improved performance.

**Response:** PID controllers are the preferred choice if the response is acceptable. We have responded to the argument of PI controllers in the discussion section of the revised manuscript.

### **Main remarks:**

1. Page 8: The sentence We assume that these three constraints are always active, meaning that the energy consumption ( $J = V$ ) is minimized by having equality for the three specifications in (3) poses a problem of understanding. In (3), there are four constraints, not three. In the previous sentence, Note that ...99.5% for the bottom product, three specifications are described. Thus, all this should be clarified.

**Response:** The referred text was confusing. We have improved this in the revised manuscript.

2. Page 22: the authors mention very briefly the use of MPC and stipulate that a linear Model Predictive Controller may not be adequate. However, all their work is done with PI controllers, thus in a linear framework. Furthermore, the handling of couplings and constraints is much more efficient with MPC because of multivariable optimization instead of simple PIs. At least, a few results of simulations in disturbance cases could have been provided with MPC.

**Response:** We have responded to this comment better in the discussion section of the revised manuscript.

### **Minor remarks:**

3. Page 1: correct as more than 100 dividing-wall columns.  
Page 3: correct studies on the divided-wall columns column.  
Page 8: correct as we may choose.  
Page 12: correct as This is quite a long story, correct that the vapor split (RV ) a degree of freedom.  
Page 12: correct liquid split vale.  
Page 16: correct The energy loop . . .were detuned, six feed composition disturbance, an equimolar nominal feed conditions.  
Page 17: correct both key impurities . . . should are controlled

**Response:**

Suggested corrections have been made.

**Reviewer # 2:**

I have read the paper "Control structure selection for three-product Petlyuk (dividing-wall) column" (CEP-D-12-00336) by Dwivedi et al. It contains some interesting material and should be published after several significant issues have been addressed. I will only address the situation in which the vapor split is fixed.

The authors use the control structure proposed by Ling and Luyben (CS3) but augment it with two override controllers that can take over the reboiler duty if too much of the lightest component is dropping out the bottom of the prefractionator side of the wall or appearing in the sidestream.

1. The feed composition disturbances are unrealistically high. Going from 33.3 mol% up to 53.3 mol% or down to 13 mol% would not be typical in any industrial situation. Ling and Luyben used feed composition disturbances of 20% relative to the design value ( from 33.3 mol% up to 40 mol% or down to 26.6 mol%). The authors should quantify how large these composition disturbances could be and still get good control from the basic CS3 without the overrides.

**Response:**

Simulations for smaller feed disturbances also show that structure CS3 fails and there is a breakthrough of light impurity (A) in the side product. The reason is that the operating point is close to a region where we may have a breakthrough of A in the side product (that is, A/B become the more difficult split even for small feed disturbance). We have responded to this comment within the revised manuscript in the discussion subsection: "Change in difficult split".

2. The authors do not tell us how they prevent "reset windup" in the three PI controllers that can alternatively manipulate reboiler duty. This should be explained in detail since it is a significant problem in override control structures.

**Response:** The "reset windup" should, in general be implemented for all PI-controllers to improve dynamic performance. We did not see a lot of deterioration in the closed loop responses as we did not change the the direction of disturbances in a single simulation run. The anti-wind may easily be implemented and is recommended for future work.

3. What deadtimes were used in the composition measurements?



**Response:** We have used SIMC rules for tuning which accounts for delay in measurements. For  $R_L$  in CS1, for example,  $\tau_C$  is 10 minutes, therefore a delay of 10 minutes may be used in principle. In this work, we did not use a delay in composition measurements though.

4. Using a logarithmic transformation in the control loops is okay for tuning purposes but showing the actual compositions in the plots would give the reader a better idea of how well the variable is being controlled. Some of the transient peak disturbances look terrible (going from 0.5 mol% impurity up to 10 mol%). That would be unacceptable in most situations. But of course smaller more realistic feed composition would give smaller disturbances.

**Response:** The choice of log-scales to show compositions was deliberate for sake of easier readability of the four compositions in a single plot.

5. Responses to increases and decreases in feed flowrate should be given. The authors state that all the schemes handle a 10% increase in feed flowrate. They should give plots that show both positive and negative 20% feed flowrate disturbances for comparison with results given by Ling and Luyben.

**Response:** We have included the closed-loop responses for  $\pm 20\%$  feed rate change in the revised manuscript. The responses are satisfactory using all the control structures for feed rate changes.